

# Analytic Treatment of Kapitza-Dirac Effect: Connecting Raman-Nath and Bragg Approximations

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## Abstract

We develop an analytical approach for probability amplitudes of Kapitza-Dirac effect that merge together the Raman-Nath and Bragg regimes of interaction.

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The Kapitza-Dirac effect constitutes diffraction of a structureless particle (electron) by a standing electromagnetic wave, exhibiting the particle-wave dual nature of matter in one of most convenient ways [1]. It appears as a counterpart to familiar optical diffraction by the periodic material grating. Matter wave of the particle beam plays the role of the incoming wave while the spatial periodicity of the grating interaction is ensured by the periodic structure of the optical standing wave potential. Since its prediction in 1933, this phenomenon was addressed theoretically many times [2, 3] and has been nicely observed experimentally by H. Batelaan et. al at Nebraska-Lincoln University [4]. (Detailed content can be found in review article [5] and dissertation [6]).

In frame of 1D model of sinusoidal periodic potential the electron wave function has a form

$$\Psi(z, t) = \sum_{n=-\infty}^{+\infty} c_n(t) \exp[i(n_0 + n)2kz] \quad (1)$$

and the problem reduces to the following difference-differential equation for  $c_n(t)$  probability amplitudes of the diffraction modes[7]:

$$\left(\frac{d}{dt} + i\omega_r(n_0 + n)^2 + iU_0\right) c_n(t) = -i\frac{U_0}{2}(c_{n-1}(t) + c_{n+1}(t)), \quad (2)$$

$n = 0, \pm 1, \pm 2, \dots$ . Here  $k$  is the wave number of the running waves which constitute the periodic potential,  $n_0 = p_{initial}/2\hbar k$  stands for the normalized electron initial momentum,  $\omega_r = E_r/\hbar$  with  $E_r = (2\hbar k)^2/2m$  is the so called recoil frequency and  $U_0$  represents the amplitude of the ponderomotive potential in  $\hbar$  units. In representation (1) the momentum transfer occurs in discrete units  $2\hbar k$  and generally is interpreted as absorption/stimulated emission of photon pairs from the counterpropagating travelling waves, which give the standing wave.

To clearly identify the limiting Raman-Nath and Bragg regimes it is convenient to introduce a new amplitude

$$C_n(t) = i^n \exp[iU_0 t + i\omega_r(n_0 + n)^2 t] c_n(t), \quad (3)$$

which transforms Eq.(2) to

$$\frac{d}{dt} C_n(t) = \frac{U_0}{2} (e^{i\omega_r(2n_0+2n-1)t} C_{n-1}(t) - e^{-i\omega_r(2n_0+2n+1)t} C_{n+1}(t)). \quad (4)$$

The analytic solution, presenting the Raman-Nath regime of interaction, corresponds to the limiting case  $\omega_r(2n_0 + 2n - 1)t \ll 2\pi$ , when the system (4) loses the time-dependent exponential coefficients, transforming into equation with first kind Bessel function solution:  $C_n(t) = J_n(U_0t)$ . Bessel function population flow of diffraction modes has a dominantly double-peaked pattern, symmetrically distributed about the initial state. This regime of realization assumes that the change of the electron position along the standing wave direction changes negligibly compared to the standing wave spatial period.

The second, Bragg regime of interaction distinguishes only discrete, equidistant values of the electron initial momentum, namely in our notations  $n_0 = \pm 1/2 \pm 1, \pm 3/2 \dots$ . Taking, for example, condition for the first order diffraction  $n_0 = -1/2$  ( $p_0 = -\hbar k$ ), one can easily see that the two amplitudes at the right hand side of system (4),  $C_0(t)$  and  $C_1(t)$ , lose the time dependence in exponential coefficients, while the other ones preserve it. Assuming now an additional condition that  $\omega_r(2n_0 + 2n - 1)t \gg 2\pi$  for any  $\omega_r$  and  $n$  (except, of course,  $n = 0, 1$ ), we get rapidly oscillating coefficients for terms  $n \neq 0, 1$  and thus almost totally suppress their contribution to the final result (it reminds the rotating wave approximation widely used in the theory of matter-laser resonance interactions). After neglecting all these terms, one arrives to a simple pair of equations

$$\frac{d}{dt}C_0(t) = -\frac{U_0}{2}C_1(t), \quad \frac{d}{dt}C_1(t) = \frac{U_0}{2}C_0(t), \quad (5)$$

resulting in  $C_0(t) = \cos(U_0t/2)$  and  $C_1(t) = \sin(U_0t/2)$  probability amplitudes for direct ( $n = 0$ ) and Bragg diffraction ( $n = 1$ ).

There is no exact analytical solution to Kapitza-Dirac problem in frame of Schrödinger equation, which will be valid for any interaction time periods and free of strict limitations on the system parameters. Diffraction regularities have analytically been treated in mentioned regimes of interaction and in close neighborhoods. They favor short- and long-time regimes respectively and are also known as the thin- and thick-crystal approximations.

In this paper we develop a theory which treats the quantum particle (electron) diffraction in the 1D periodic potential for any times of interaction. Our formula quantitatively correctly describes both Raman-Nath and Bragg regimes of interaction, thereby merging them into one essence of diffraction process.

Our approach to the infinite system of equations (2) originates from the remark that it connects the seeking amplitudes with opposite parity on the left hand and right hand sides

of the equations. Initial condition  $c_n(0) = \delta_{n,0}$  is, however, different for these two families of amplitudes: all odd ones are zeroes, while the only nonzero member sits in the even-manifold. Any approximate solution should be sensitive to the initial conditions too, as we get rid of one of the parities in the set of equations by introducing new, phase-shifted amplitudes

$$\overline{c}_n(t) = i^n \exp[iU_0 t] c_n(t) \quad (6)$$

and arriving to

$$\begin{aligned} & \left( \frac{d}{dt} + i\omega_r ((n_0 + n)^2 + 1) \right)^2 \left( \frac{d}{dt} + i\omega_r (n_0 + n)^2 \right) \overline{c}_n(t) + \\ & \left( 4\omega_r^2 (n_0 + n)^2 \left( \frac{d}{dt} + i\omega_r (n_0 + n)^2 \right) + \frac{U_0^2}{2} \left( \frac{d}{dt} + i\omega_r ((n_0 + n)^2 + 1) \right) \right) \overline{c}_n(t) \\ & = \frac{U_0^2}{2} \left( \frac{d}{dt} + i\omega_r ((n_0 + n)^2 + 1)^2 \right) (\overline{c}_{n-2}(t) + \overline{c}_{n+2}(t)). \end{aligned} \quad (7)$$

It preserves the original tridiagonal form of (2) but is now a third order differential - difference equation. In the following treatment the set (7) will be regarded to describe the even-manifold of amplitudes.

We look for a trial solution of a definite integral form

$$\overline{c}_n(t) = \exp[-i\omega_r (n_0 + n)^2 t] \frac{(-i)^n}{\pi} \int_0^\pi \cos(n\varphi) \exp[i\lambda_n(\varphi)t] d\varphi, \quad (8)$$

where the  $n$ -dependent function  $\lambda_n(\varphi)$  has to be determined yet. Inserting Eq.(8) into (7) we obtain the following three difference algebraic equations:

$$\lambda_{n-2}(\varphi) + 4\omega_r (n_0 + n - 1) - \lambda_n(\varphi) = 0 \quad (9)$$

$$\lambda_{n+2}(\varphi) + 4\omega_r (n_0 + n + 1) - \lambda_n(\varphi) = 0 \quad (10)$$

$$\begin{aligned} & \left( (\lambda_n(\varphi) + \omega_r)^2 \lambda_n(\varphi) - 4\omega_r^2 (n_0 + n)^2 \lambda_n(\varphi) - \frac{U_0^2}{2} (\lambda_n(\varphi) + \omega_r) \right) \cos(n\varphi) \\ & = \frac{U_0^2}{4} (\lambda_{n-2}(\varphi) + \omega_r (6n_0 + 6n - 3)) \cos((n-2)\varphi) + \frac{U_0^2}{4} (\lambda_{n+2}(\varphi) - \omega_r (2n_0 + 2n - 3)) \cos((n+2)\varphi). \end{aligned} \quad (11)$$

Hence, for the trial function to be an exact solution of Eq.(7), the Eqs. (9)-(11) should be identical to each other. Eq. (9) and (10) are really mutually equivalent and one of them, for instance Eq. (9), can be put out from consideration. The last one, Eq. (11), however, is not equivalent to Eqs. (9) and (10). This means that the analytic form (8) can not be an exact solution to the problem. Our approximation lies just in this point and amounts

to taking of Eqs. (9)-(11) as a system of three equations relative to  $\lambda_{n+2}(\varphi)$ ,  $\lambda_{n-2}(\varphi)$  and seeking  $\lambda_n(\varphi)$ . Then finding  $\lambda_{n+2}(\varphi)$  as a linear function of  $\lambda_n(\varphi)$  and inserting it into Eq. (11), we arrive to a third order algebraic equation

$$(\lambda_n(\varphi) + 2\omega_r/3)^3 + p_n(\varphi)(\lambda_n(\varphi) + 2\omega_r/3) + q_n(\varphi) = 0 \quad (12)$$

with real coefficients

$$p_n(\varphi) = -\left(U_0^2 \cos^2(\varphi) + 4\omega_r^2(n_0 + n)^2 + \omega_r^2/3\right)$$

and

$$q_n(\varphi) = -\frac{2}{27}\omega_r^3 - U_0^2\omega_r \left(\frac{1}{3}\cos^2(\varphi) + (n_0 + n)\cos(2\varphi)\right) + \frac{8}{3}\omega_r^3(n_0 + n)^2.$$

The sign of the first coefficient is always negative and depending on the sign of quantity

$$Q_n(\varphi) = \left(\frac{p_n(\varphi)}{3}\right)^3 + \left(\frac{q_n(\varphi)}{2}\right)^2$$

one has two distinct forms for the solutions of Eq. (12)[8].

Later on we'll denote the three roots of Eq. (12) as  $\lambda_n(j; \varphi)$ ,  $j = 1, 2, 3$ , the corresponding amplitudes as  $\overline{c}_n(j; t)$  and the respective wave functions as  $\Psi(j; z, t)$ . Then the general form of probability amplitudes should be written as

$$\Psi(z, t) = h_1\Psi(1; z, t) + h_2\Psi(2; z, t) + h_3\Psi(3; z, t) \quad (13)$$

or, equivalently

$$c_n(t) = \exp[-i\omega_r(n_0 + n)^2 t - iU_0 t] \frac{(-1)^n}{\pi} \times \int_0^\pi (h_1 \exp[i\lambda_n(1; \varphi)t] + h_2 \exp[i\lambda_n(2; \varphi)t] + h_3 \exp[i\lambda_n(3; \varphi)t]) \cos(n\varphi) d\varphi. \quad (14)$$

Three  $h$ -coefficients are determined from initial conditions for the wave function (13) and its first and second derivatives:

$$\begin{aligned} h_1 + h_2 + h_3 &= 1, \\ l_1 h_1 + l_2 h_2 + l_3 h_3 &= 0, \\ L_1 h_1 + L_2 h_2 + L_3 h_3 &= U_0^2/2, \end{aligned} \quad (15)$$

with the following notations for coefficients:

$$l_j = \frac{1}{\pi} \int_0^\pi \lambda_{n=0}(j; \varphi) d\varphi, \quad L_j = \frac{1}{\pi} \int_0^\pi \lambda_{n=0}(j; \varphi)^2 d\varphi, \quad (16)$$

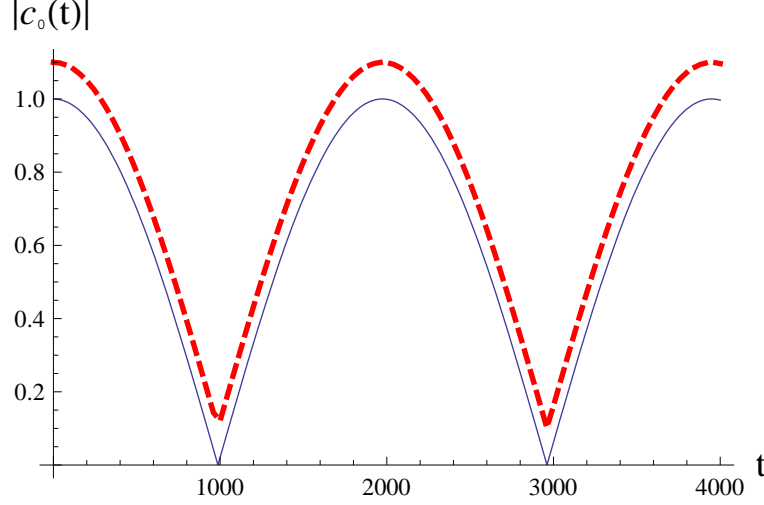


FIG. 1: (Color online)  $n = 0$  diffraction probability amplitude evolution in Bragg diffraction regime. Solid line gives the result of exact numerical simulation. Dashed line is the amplitude evolution for analytic formula described in the text. The dashed line is shifted vertically by 0.1 to make the two lines visually different (we will make this shift in all figures). Horizontal time axis is normalized to green light ( $\lambda_{green} = 6000\text{\AA}$ ) Compton backscattering frequency shift  $\Delta\omega_{Compton} = 4\pi\hbar\omega_{green}^2/M_e c^2$ , where  $M_e$  is the electron mass. Other parameters are  $n_0 = -0.5$ ,  $U_0 = 0.01\Delta\omega_{Compton}/\pi$ ,  $\omega_r = \Delta\omega_{Compton}/\pi$ .

$j = 1, 2, 3$ . This step crowns the procedure and hence the formula (14) presents the solution of the problem for any even  $n$ , the amount of acquired momentum in  $2\hbar k$  units.

To determine still untouched odd- probability amplitudes, we have to return to original equation (1) and shift the numbering by one:

$$\left(\frac{d}{dt} + i\omega_r(n_0 + n)^2 + iU_0\right)c_{n+1}(t) = -i\frac{U_0}{2}(c_n(t) + c_{n+2}(t)), \quad (17)$$

Inserting even- $n$  solutions into the right hand side of (17) and simply integrating equation with zero initial condition, we complete our approach to analytic solution of the stated Kapitza-Dirac diffraction problem.

To value the developed analytic approximation, we have compared its results with the exact numerical solutions of the original set of Eqs. (2). In order to implement these simulations we have used the Crank-Nicolson method [9]. Comparison shows that the presented approximation works excellent in both, Raman-Nath and Bragg regimes of interaction. Two particular cases are illustrated in Figs.1-4. The graphs in each figure are indistinguishable

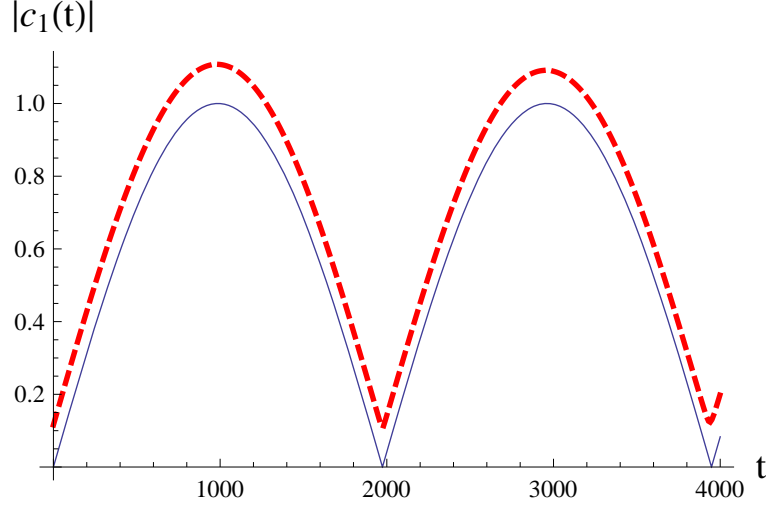


FIG. 2: (Color online)  $n = 1$  diffraction probability amplitude evaluation in Bragg diffraction regime. All the parameters are as in Fig.1.

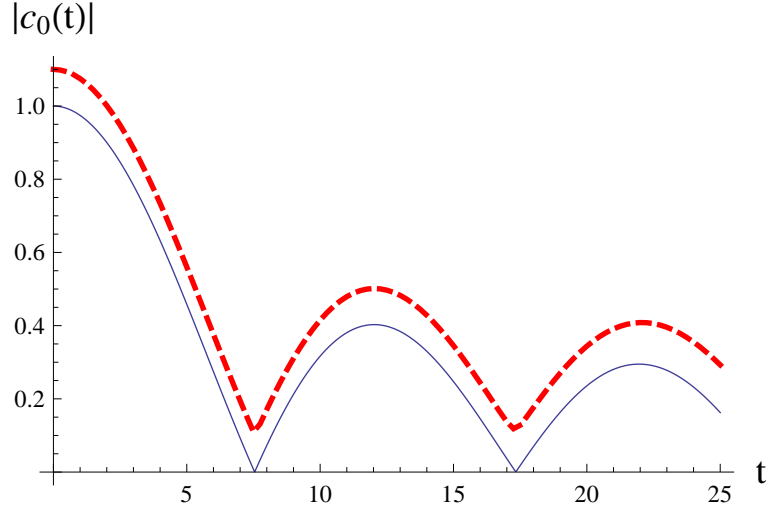


FIG. 3: (Color online)  $n = 0$  diffraction probability amplitude evaluation in Raman-Nath diffraction regime.  $n_0 = -0.5$ ,  $U_0 = \Delta\omega_{Compton}/\pi$ ,  $\omega_r = 0.001\Delta\omega_{Compton}/\pi$ .

from each other at sight and are shifted in vertical direction in illustrative purposes.

In intermediate regimes (relative to Raman-Nath and Bragg) our numerical calculation has definite restrictions, connected with the limitations on calculation of inverse matrices required by the Crank-Nicolson method. Thus ultimate conclusions here cant be done yet. However, every case when we were sure in the correctness of numerical calculations

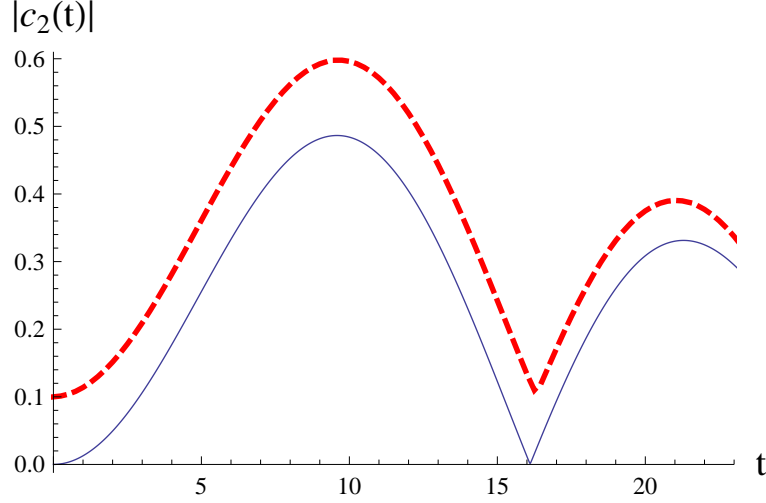


FIG. 4: (Color online)  $n = 2$  diffraction probability amplitude evaluation in Raman-Nath diffraction regime. All the parameters are as in Fig.3.

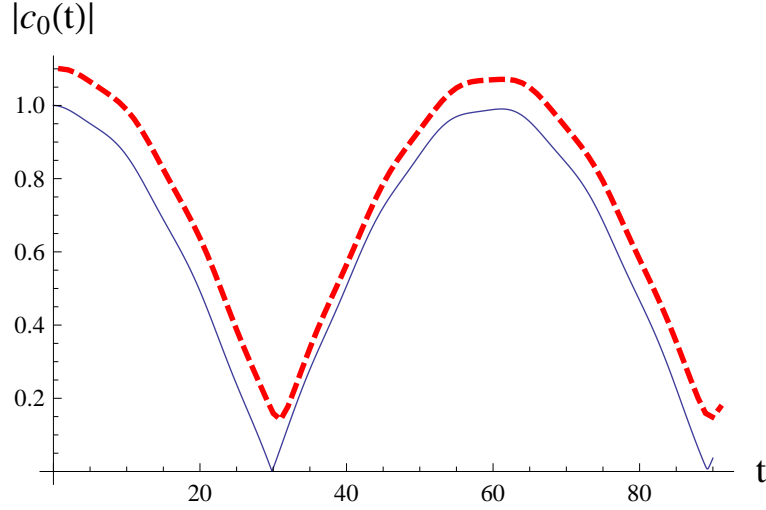


FIG. 5: (Color online)  $n = 0$  diffraction probability amplitude evaluation in intermediate diffraction regime.  $n_0 = -0.5$ ,  $U_0 = \Delta\omega_{Compton}/3\pi$ ,  $\omega_r = \Delta\omega_{Compton}/\pi$ .

the coincidence between our approximate analytical results and numerical ones was quiet good. Fig. 5 and 6 illustrate such a case with parameter values  $U_0 \approx \omega_r$  (note that the Raman-Nath approximation requires  $U_0 \gg \omega_r$ , and the Bragg approximation - the opposite one  $U_0 \ll \omega_r$ ).

This gives some credibility to the presented analytical approximation over the intermedi-



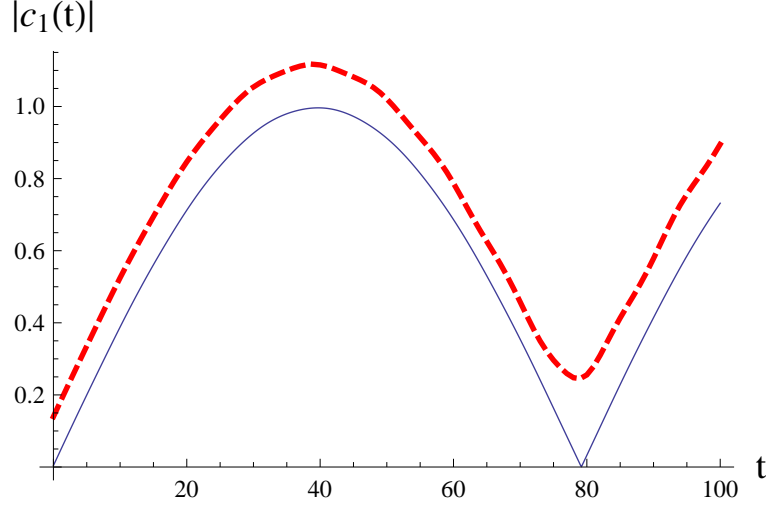


FIG. 6: (Color online)  $n = 1$  diffraction probability amplitude evolution in intermediate diffraction regime.  $n_0 = -0.5$ ,  $U_0 = \Delta\omega_{Compton}/4\pi$ ,  $\omega_r = \Delta\omega_{Compton}/\pi$ .

ate range of parameters too and in the future we will endeavour in reaching a full definiteness in this direction too.

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